isoprocarb, TFA

Inchi: InChI=1S/C13H14F3NO3/c1-8(2)9-6-4-5-7-10(9)20-12(19)17(3)11(18)13(14,15)16/h4-8H
InchiKey: PVKANSNDYAANOM-UHFFFAOYSA-N
Formula: C13H14F3NO3
SMILES: CC(C)c1ccccc1OC(=O)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 289.25

Physical Properties

Property code	Value	Unit	Source
gf	-674.73	kJ/mol	Joback Method
hf	-978.80	kJ/mol	Joback Method
hfus	28.79	kJ/mol	Joback Method
hvap	61.28	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.329		Crippen Method
mcvol	194.570	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	665.24	K	Joback Method
tc	862.20	K	Joback Method
tf	418.96	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.46	J/mol×K	665.24	Joback Method
cpg	540.82	J/mol×K	698.07	Joback Method
cpg	553.27	J/mol×K	730.89	Joback Method
cpg	564.84	J/mol×K	763.72	Joback Method
cpg	575.59	J/mol×K	796.54	Joback Method
cpg	585.55	J/mol×K	829.37	Joback Method

cpg	594.76	J/mol×K	862.20	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume